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=> fil reg
FILE 'REGISTRY' ENTERED AT 09:19:56 ON 23 MAY 2006
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STRUCTURE FILE UPDATES:   22 MAY 2006  HIGHEST RN 885262-53-3
DICTIONARY FILE UPDATES:  22 MAY 2006  HIGHEST RN 885262-53-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
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Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d sta que l26
L12             STR

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     ||
Cy---C---CH2---CH2---NH---Ak
1   2   3     5     6    7


NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   7

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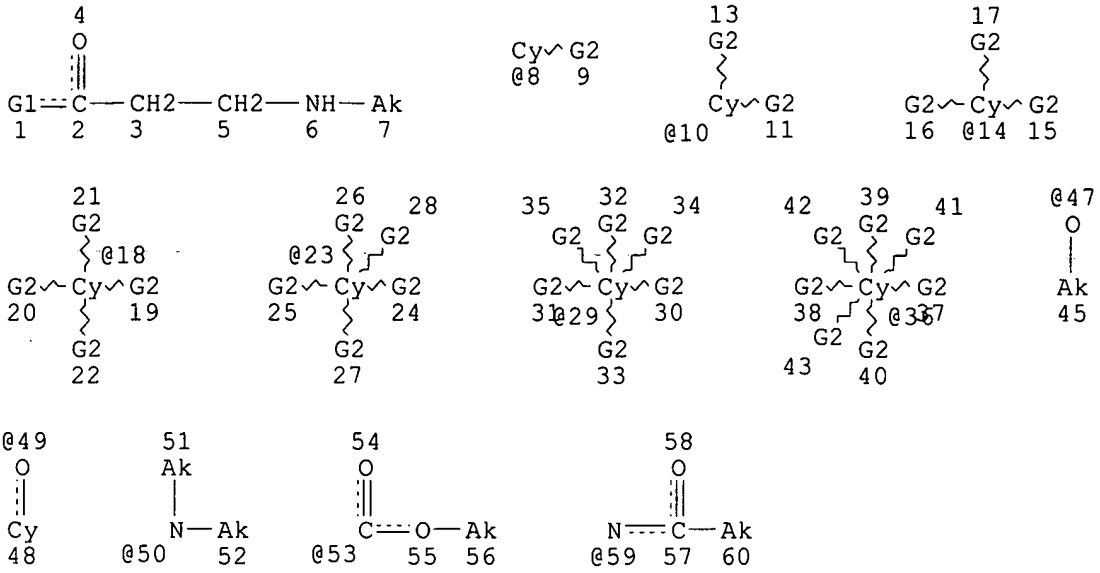

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STEREO ATTRIBUTES: NONE
L26 297 SEA FILE=REGISTRY SUB=L16 CSS FUL L24

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SEARCH TIME: 00.00.04

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(FILE 'HOME' ENTERED AT 08:54:36 ON 23 MAY 2006)
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FILE 'HCAPLUS' ENTERED AT 08:54:46 ON 23 MAY 2006
L1 1 S (WO2003-EP8514 OR DE2002-10240026)/AP,PRN
E FABIAN/AU
E FABIAN K/AU
L2 24 S E3-E5
E NIESERT/AU
L3 15 S E7-E9
E KRALIK/AU
L4 30 S E33-E35,E42
E GLUSENKAMP/AU
L5 6 S E4,E5
SEL RN L1

FILE 'REGISTRY' ENTERED AT 08:56:37 ON 23 MAY 2006
L6 4 S E1-E4

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L7            2 S L6 NOT (CH2O OR C6H6OS)
L8            3 S 27152-62-1/CRN
L9            6 S 667465-15-8/CRN
L10           3 S L9 NOT COMPD
L11           8 S L7,L8,L10
L12             STR
L13           1 S L12 CSS SAM
L14             SCR 1597
L15           8 S L12 AND L14 CSS SAM
L16         570 S L12 AND L14 CSS FUL
                SAV TEMP L16 SHA525/A
L17          21 S L16 AND SC4/ES
L18          15 S L17 AND 1/NR
L19           6 S L17 NOT L18
                SEL RN 4-6
L20           3 S L19 NOT E5-E7
L21          18 S L18,L20
L22         239 S L16 AND 46.150.18/RID
L23         169 S L22 AND 1/NR
L24             STR L12
L25          10 S L24 CSS SAM SUB=L16
L26         297 S L24 CSS FUL SUB=L16
                SAV TEMP L26 SHA525A/A
L27         296 S L26/COM
L28          19 S L17 AND L27
L29           1 S L28 NOT L21
L30          18 S L28 NOT L29
L31          18 S L21,L30
L32         128 S L27 AND 46.150.18/RID
L33         112 S L32 AND 1/NR
L34         111 S L33 NOT MAN/CI
L35         129 S L31,L34
L36          15 S L32 NOT L35
L37          14 S L36 NOT MAN/CI
L38         143 S L35,L37
L39             STR L24
L40           4 S L39 CSS SAM SUB=L27
L41         158 S L39 CSS FUL SUB=L27
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L42         272 S L38,L41
                SAV TEMP L42 SHA525C/A
L43          25 S L26 NOT L42
L44         264 S L42 NOT L11

     FILE 'HCAOLD' ENTERED AT 09:16:27 ON 23 MAY 2006
L45           3 S L11
                SEL AN
                EDIT E8-E10 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 09:16:55 ON 23 MAY 2006
L46           6 S E8-E10
L47           3 S L46 NOT (CARLIN ? OR SOKOLOV ? OR GRAFE ?)/AU
L48          36 S L11
L49          36 S L47,L48
L50          29 S L49 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L51           2 S L49 AND L1-L5
L52           2 S L49 AND MERCK?/PA,CS
L53          18 S L11(L)PREP+NT/RL
L54          12 S L50 AND L53
L55          13 S L51,L52,L54
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L56          16 S L50 NOT L55
L57          29 S L55,L56

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FILE COVERS 1907 - 23 May 2006  VOL 144 ISS 22
FILE LAST UPDATED: 22 May 2006  (20060522/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d l57 bib abs hitstr retable tot

L57  ANSWER 1 OF 29  HCAPLUS  COPYRIGHT 2006 ACS on STN
AN   2004:308427  HCAPLUS
DN   140:321232
TI   Preparation of optically active 3-amino-1-(2-thienyl)-1-propanols via
     reduction of 3-amino-1-(2-thienyl)-1-propanones using a hydrogen donor in
     the presence of a metal catalyst, an optically active nitrogen-containing
     ligand and optionally a base.
IN   Fuchs, Rudolf; Michel, Dominique; Brieden, Walter
PA   Lonza A.-G., Switz.
SO   PCT Int. Appl., 25 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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PI   WO 2004031168        A2    20040415    WO 2003-EP11073        20031007 <--
     WO 2004031168        A3    20040826
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
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             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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AU 2003276066 A1 20040423 AU 2003-276066 20031007 <--
PRAI EP 2002-22540 A 20021007 <--
WO 2003-EP11073 W 20031007
OS CASREACT 140:321232; MARPAT 140:321232
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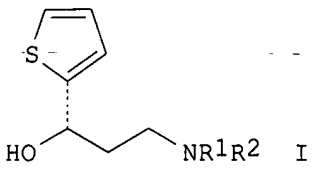

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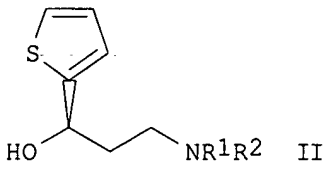
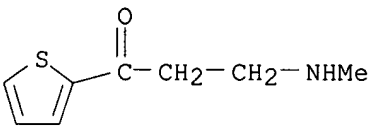


II

AB Title compds. (I, II; R1, R2 = H, alkyl, cycloalkyl, aralkyl, aryl), were prepared by reducing the corresponding 3-amino-1-(2-thienyl)-1-propanones using a hydrogen donor in the presence of a metal catalyst, an optically active N-containing ligand and optionally a base. Thus, 3-N-methylamino-1-(2-thienyl)-1-propanone hydrochloride (preparation given) and NaOH were stirred 1 h in Me2CHOH; a prestirred solution of (1S,2R)-cis-1-amino-2-indanol and (p-cymene)ruthenium(II)chloride dimer in Me2CHOH was added followed by stirring for 4 h at 20° to give 39% (S)-N-methylamino-1-(2-thienyl)-1-propanol in 70% enantiomeric excess.

IT **645411-16-1P**, 3-N-Methylamino-1-(2-thienyl)-1-propanone hydrochloride
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of optically active aminothienylpropanols via reduction of aminothienylpropanones using a hydrogen donor in the presence of a metal catalyst, an optically active N-containing ligand and a base)

RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)




● HCl

L57 ANSWER 2 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:203795 HCAPLUS
DN 140:253262
TI Method for the preparation amino alcohols via the enantioselective hydrogenation of amino ketones
IN **Kralik, Joachim; Fabian, Kai**; Muermann, Christoph; Schweickert, Norbert
PA **Merck Patent G.m.b.H., Germany**
SO PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DT Patent

LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2004020389 | A1 | 20040311 | WO 2003-EP8513 | 20030801 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2496883 | AA | 20040311 | CA 2003-2496883 | 20030801 |
| | AU 2003260347 | A1 | 20040319 | AU 2003-260347 | 20030801 |
| | EP 1532100 | A1 | 20050525 | EP 2003-790842 | 20030801 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| | BR 2003013795 | A | 20050712 | BR 2003-13795 | 20030801 |
| | CN 1678562 | A | 20051005 | CN 2003-820304 | 20030801 |
| | JP 2005536556 | T2 | 20051202 | JP 2004-531845 | 20030801 |
| | US 2005261514 | A1 | 20051124 | US 2005-525821 | 20050225 |
| | ZA 2005002458 | A | 20051010 | ZA 2005-2458 | 20050324 |
| PRAI | DE 2002-10240025 | A | 20020827 | | |
| | WO 2003-EP8513 | W | 20030801 | | |

OS CASREACT 140:253262; MARPAT 140:253262
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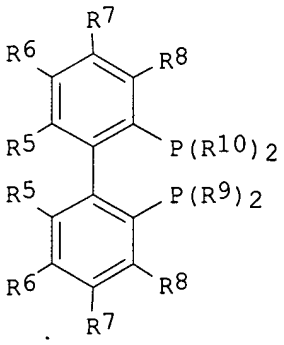


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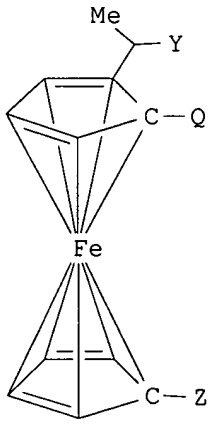


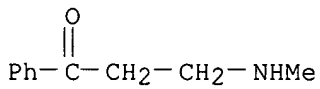

II

AB The invention relates to methods for the enantioselective production of amino alcs., R1CH(OH)CH2(CH2)nNHR2 [R1 = (un)substituted, (un)saturated or aromatic carbocycle or heterocycle (optionally substituted with R3, R4); R2 = H, C1-20-alkyl; R3, R4 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, CO2R2, F, Cl, Br, OH, CN,NO2,N(R2)2, NHCOR2; n = 0 - 3], via the enantioselective hydrogenation of amino ketones, R1COCH2(CH2)nNHR2 and is characterized by

hydrogenation in the presence of a non-racemic catalyst containing a chiral diphosphine ligand I [R5, R6, R7, R8 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, F, Cl, Br,N(R2)2, NHCOR2; R5R6, R6R7, R7R8 = (CH2)4, CH:CHCH:CH,etc.; R9, R10 = C6H4(R11)m, 2-furyl, cyclohexyl; R11 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, SO3Na, COR12, F, Cl, N(R12)2, NHCOR12; R12 = H, C1-20-alkyl; m = 0 - 3] or II [Q = PPh2, P(cyclohexyl)2, P[C6H3(CF3)2-3,5], P(4-methoxy-3,5-dimethylphenyl)2, P(CMe3)2; Y = OH, P(cyclohexyl)2, P(C6H3Me2-3,5)2, P(CMe3)2; Z = H, PPh2; Ph = unsubstituted Ph, C6H4Me-2, C6H4Me-3, C6H4Me-4, C6H3Me2]. Thus, (S)-N-methyl-3-hydroxy-3-(2-thienyl)propanamine was prepared with 92.8% e.e. from 3-(methylamino)-1-(2-thienyl)-1-propanone via asym. hydrogenation in MeOH/PhMe containing catalytic bis(1,5-cyclooctadiene)dirhodium(I) dichloride and (S)-(-)-2,2'-bis[di(p-tolyl)phosphine]-1,1'-binaphthyl.

IT **27152-62-1**, 3-(Methylamino)-1-phenyl-1-propanone
**667465-15-8**, 3-(Methylamino)-1-(2-thienyl)-1-propanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective hydrogenation of; preparation amino alcs. via the enantioselective hydrogenation of amino ketones with chiral diphosphine ligands)

RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



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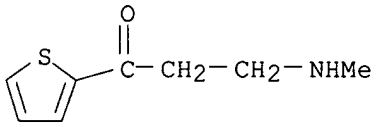

RETABLE

| Referenced Author (RAU) | Year (RPY) | VOL (RVL) | PG (RPG) | Referenced Work (RWK) | Referenced File |
|---|---|---|---|---|---|
| Helmchen, G | 1995 | E21d | 3955 | HOUBEN-WEYL METHODS | |
| Kitamura, M | 1998 | 110 | 629 | J AM CHEM SOC | |

L57 ANSWER 3 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:198214 HCAPLUS
DN 140:235592
TI Process for the preparation of monoalkylaminoethyl aryl ketones from bis(arylcarbonylethyl)alkylamines.
PA **Merck Patent G.m.b.H., Germany**
SO Ger. Offen., 7 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI DE 10240026 | A1 | 20040311 | DE 2002-10240026 | 20020827 <-- |

CA 2497028 AA 20040311 CA 2003-2497028 20030801 <--
WO 2004020391 A1 20040311 WO 2003-EP8514 20030801 <--
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AU 2003260348 A1 20040319 AU 2003-260348 20030801 <--
EP 1532101 A1 20050525 EP 2003-790843 20030801 <--
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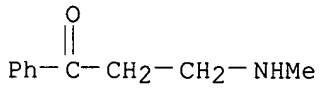
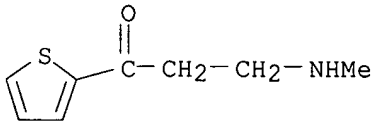
BR 2003013796 A 20050927 BR 2003-13796 20030801 <--
CN 1678564 A 20051005 CN 2003-820305 20030801 <--
JP 2005536557 T2 20051202 JP 2004-531846 20030801 <--
PRAI DE 2002-10240026 A 20020827 <--
WO 2003-EP8514 W 20030801 <--
OS CASREACT 140:235592; MARPAT 140:235592
AB R1COCH2CH2NHR2 [R1 = (substituted) (unsatd.) residue, aromatic heterocyclyl; R2 = alkyl], were prepared by reaction of R1COCH2CH2NR2CH2CH2COR1 (variables as above) with R2NH2.
IT **27152-62-1P 667465-15-8P**
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(preparation of monoalkylaminoethyl aryl ketones from bis(arylcarbonylethyl)alkylamines)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



RN 667465-15-8 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)- (9CI) (CA INDEX NAME)



L57 ANSWER 4 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:41488 HCAPLUS
DN 140:93915
TI Process for the preparation of optically active 3-N-methylamino-1-(2-thienyl)-1-propanol
IN Michel, Dominique
PA Lonza A.-G., Switz.
SO PCT Int. Appl., 34 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI | WO 2004005307 | A1 | 20040115 | WO 2003-EP7312 | 20030708 <-- |
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| | AU 2003253036 | A1 | 20040123 | AU 2003-253036 | 20030708 <-- |
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OS CASREACT 140:93915; MARPAT 140:93915
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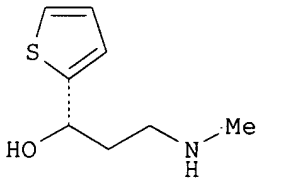

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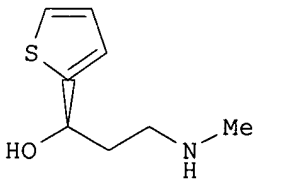

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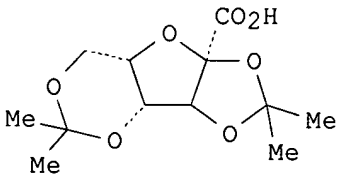
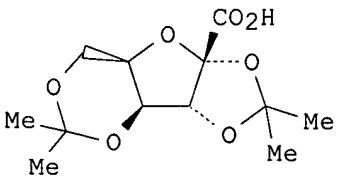


III

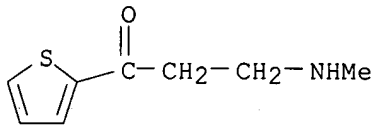


IV

AB Enantiomerically enriched (S)-(-)-3-N-methylamino-1-(2-thienyl)-1-propanol (I) or (R)-(+)-3-N-methylamino-1-(2-thienyl)-1-propanol (II) or mirror image are prepared by (i) treating an enantiomeric mixture of the amines I and II with (-)-2,3:4,6-di-O-isopropylidene-2-keto-L-gulonic acid (III) or (+)-2,3:4,6-di-O-isopropylidene-2-keto-D-gulonic acid (IV), (ii) crystallizing the obtained diastereomerically enriched salts from the reaction mixture obtained in step (i), (iii) optionally recrystg. said diastereomerically enriched salts I.III or II.IV, and (iv) treating the diastereomerically enriched salts II.III or II.IV obtained in step (ii) or step (iii) with a base to liberate the enantiomerically enriched amines I or II.

IT **645411-16-1P**, 3-(N-Methylamino)-1-(2-thienyl)-1-propanone hydrochloride
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of optically active N-methylamino(thienyl)propanol by optical resolution via formation of diastereomer salts with 2,3:4,6-di-O-isopropylidene-2-ketogulonic acid)

RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RETABLE

| Referenced Author (RAU) | Year (RPY) | VOL (RVL) | PG (RPG) | Referenced Work (RWK) | Referenced File |
|---|---|---|---|---|---|
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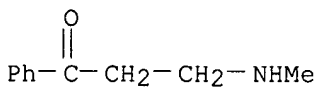
| Fitzi, R | 1988 | 44 | 5277 | TETRAHEDRON | HCAPLUS |
| Robertson, D | 1991 | | | US 5023269 A | HCAPLUS |
| William Den, H | 1972 | | | US 3682925 A | HCAPLUS |

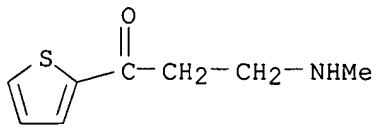
L57 ANSWER 5 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:41430 HCAPLUS
DN 140:93914
TI Process for the preparation of N-monosubstituted β-amino alcohols
IN Michel, Dominique
PA Lonza A.-G., Switz.
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2004005239 | A1 | 20040115 | WO 2003-EP7411 | 20030709 <-- |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2491472 | AA | 20040115 | CA 2003-2491472 | 20030709 <-- |
| | AU 2003250924 | A1 | 20040123 | AU 2003-250924 | 20030709 <-- |
| | BR 2003012651 | A | 20050426 | BR 2003-12651 | 20030709 <-- |
| | EP 1539673 | A1 | 20050615 | EP 2003-762669 | 20030709 <-- |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| | CN 1665773 | A | 20050907 | CN 2003-816223 | 20030709 <-- |
| | JP 2005532383 | T2 | 20051027 | JP 2004-518758 | 20030709 <-- |
| | NO 2005000079 | A | 20050311 | NO 2005-79 | 20050106 <-- |
| | US 2005256318 | A1 | 20051117 | US 2005-520362 | 20050418 |
| PRAI | EP 2002-15229 | A | 20020709 <-- | | |

WO 2003-EP7411 W 20030709
OS CASREACT 140:93914; MARPAT 140:93914
AB The invention relates to a process for the synthesis of N-monosubstituted β-amino alcs. of formula HOCH(R1)CH2CH2NHR2 and/or an addition salt of a proton acid (wherein R1 and R2 independently represent alkyl, cycloalkyl, aryl or aralkyl, each being optionally further substituted with alkyl, alkoxy and/or halogen) via direct preparation of N-monosubstituted β-amino ketones of R1COCH2CH2NHR2 and its addition salts of proton acids (wherein R1 and R2 are as defined above). Thus, 2-acetylthiophene 25.5, methylamine hydrochloride 14.9, paraformaldehyde 8.2, concentrated HCl 1.0 g, 100 mL ethanol were heated in an autoclave at 110° and a total pressure of 2-2.5 bar for 9 h, followed by removing 50 mL ethanol in vacuo and addition of 200 mL Et acetate under vigorous stirring, and filtration to give 71% 3-(methylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride (I). To a mixture of 10.3 g I and 35 mL ethanol at 4° sodium hydroxide (4.0 g of a 50% aqueous solution) was added in about 5 min and afterwards, 0.95 g neat sodium borohydride in several portions in about 30 min. The resulting suspension was stirred for 4 h at the same temperature, treated dropwise with 10.0 mL acetone in 5 min, stirred for 10 addnl. minutes, treated with 20 mL H2O, concentrated about 5 times under vacuum, and extracted with tert-Bu Me ether (2 x 20 mL). The collected organic phases were finally concentrated under vacuum affording an orange oil which crystallized spontaneously after a few hours to give 3-(methylamino)-1-(thiophen-2-yl)propan-1-ol as an orange solid (7.2 g, 84 % yield).
IT **2538-50-3P**, 3-(Methylamino)-1-phenylpropan-1-one hydrochloride
**645411-16-1P**, 3-(Methylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; process for preparation of N-monosubstituted β-amino alcs. by reduction of N-monosubstituted β-amino ketones)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RETABLE

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| Kiyoshi, M | 1982 | 94 | 937 | ANGEWANDTE CHEMIE | |
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| Lewis, W | 1958 | 47 | 77 | JOURNAL OF THE AMERI | |
| Lilly Co Eli | 1991 | | | EP 0457559 A | HCAPLUS |
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| Saldabols, N | 1962 | 2 | 309 | LATVIJAS PSR ZINATNU | |
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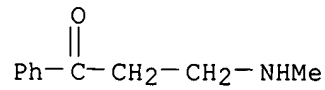
L57 ANSWER 6 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:283018 HCAPLUS
DN 137:78622
TI Oxidative reactions of azines. 9. Cascade and stage oxidation of 1,4-disubstituted 1,2,3,6-tetrahydropyridines by potassium permanganate
AU Soldatenkov, A. T.; Temesgen, A. V.; Bekro, I. A.
CS Russian Peoples Friendship University, Moscow, 117193, Russia
SO Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (**2001**), 37(10), 1216-1222
CODEN: CHCCAL; ISSN: 0009-3122
PB Kluwer Academic/Consultants Bureau
DT Journal
LA English
OS CASREACT 137:78622
AB A general scheme was developed for the cascade and stage oxidation of 1,4-disubstituted 1,2,3,6-tetrahydropyridines by potassium permanganate, based on the successive oxidation of the allylic triad of carbon atoms in the piperidine ring. In the case of 4-aryltetrahydropyridines 2-oxotetrahydropyridines are formed initially. 3,4-Dihydroxypiperidin-2-ones and finally 1-aminoalkan-3-ones are then formed. The oxidation of 4-methyl-substituted tetrahydropyridines to the analogous 1-aminoalkanones begins differently - with 3,4-dihydroxylation followed by lactamization of the piperidinediols.
IT **27152-62-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(cascade and stage oxidation of 1,4-disubstituted 1,2,3,6-tetrahydropyridines by potassium permanganate)

RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



RETABLE

| Referenced Author (RAU) | Year (RPY) | VOL (RVL) | PG (RPG) | Referenced Work (RWK) | Referenced File |
|---|---|---|---|---|---|
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| Korshunov, S | 1966 | 35 | 2255 | Usp Khim | HCAPLUS |
| Maksimova, T | 1980 | | 783 | Khim Geterotsikl Soe | HCAPLUS |
| Shinohara, T | 1997 | 45 | 813 | Chem Pharm Bull | HCAPLUS |
| Soldatenkov, A | 1996 | | 222 | Khim Geterotsikl Soe | HCAPLUS |
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| Soldatenkov, A | 2001 | | 916 | Khim Geterotsikl Soe | |
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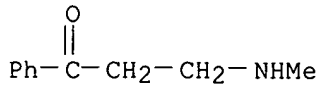
| Soldatenkov, A | 1998 | | 137 | Mendeleev Commun | HCAPLUS |
| Soldatenkov, A | 1998 | | 193 | Mendeleev Commun | HCAPLUS |
| Soldatenkov, A | 1997 | | 2020 | Ser Khim | |

L57 ANSWER 7 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:683252 HCAPLUS
DN 134:21369
TI Identification and Comparison of Impurities in Fluoxetine Hydrochloride Synthesized by Seven Different Routes
AU Wirth, David D.; Miller, Marybeth S.; Boini, Sathish K.; Koenig, Thomas M.
CS Lilly Research Laboratories, Eli Lilly and Co., Lafayette, IN, 47909-9201, USA
SO Organic Process Research & Development (**2000**), 4(6), 513-519
CODEN: OPRDFK; ISSN: 1083-6160
PB American Chemical Society
DT Journal
LA English
AB Fluoxetine-HCl was prepared by seven different synthetic routes, all previously reported. The major impurities in each route were identified by GC/MS, HPLC/MS, and gradient HPLC anal. Impurities were classified as being derived from impurities in 4-chlorobenzotrifluoride, those arising during the SNAr reaction of this compound and 3-methylamino-1-phenylpropanol, and those arising during the synthesis of this alc. Fifteen impurities belonging to the latter two categories were identified, and their structures were confirmed by synthesis of authentic material for most of the compds. It was found that a variety of anal. tools was needed for complete characterization of the impurity profile of fluoxetine HCl and that purification of the intermediate and recrystn. of the drug itself are highly effective in minimizing the levels of the impurities.
IT **27152-62-1P**
RL: **BYP (Byproduct); PREP (Preparation)**
(impurities in fluoxetine hydrochloride synthesized by seven different routes)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



RETABLE

| Referenced Author (RAU) | Year (RPY) | VOL (RVL) | PG (RPG) | Referenced Work (RWK) | Referenced File |
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| Crnic, Z | 1997 | | | US 5618968 | HCAPLUS |
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| Kuehne, M | 1977 | 42 | 2082 | J Org Chem | HCAPLUS |
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| Maryanoff, B | 1985 | 107 | 21726 | J Am Chem Soc | |
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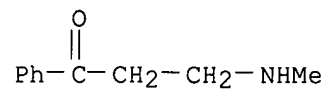
| Parli, C | 1974 | 33 | 560 | Fed Proc | |
| Perrine, D | 1998 | 75 | 1266 | J Chem Educ | HCAPLUS |
| Reiter, J | 1988 | | | WO 9811054 | HCAPLUS |
| Robertson, D | 1988 | 31 | 1412 | J Med Chem | HCAPLUS |
| Sakuraba, S | 1995 | 43 | 748 | Chem Pharm Bull | HCAPLUS |
| Schwartz, E | 1993 | | | US 5225585 | HCAPLUS |
| Theriot, K | 1998 | | | US 5760243 | HCAPLUS |
| Wirth, D | 1997 | 46 | 511 | Chromatographia | HCAPLUS |
| Wirth, D | 1997 | 1 | 55 | Org Process Res Dev | HCAPLUS |

L57 ANSWER 8 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:26204 HCAPLUS
DN 128:132529
TI Screening methods for impurities in multi-sourced fluoxetine hydrochloride drug substances and formulations
AU Wirth, D. D.; Olsen, B. A.; Hallenbeck, D. K.; Lake, M. E.; Gregg, S. M.; Perry, F. M.
CS Lilly Research Laboratories, Eli Lilly Co., Lafayette, IN, 47902, USA
SO Chromatographia (**1997**), 46(9/10), 511-523
CODEN: CHRGB7; ISSN: 0009-5893
PB Friedrich Vieweg & Sohn Verlagsgesellschaft mbH
DT Journal
LA English
AB Gradient HPLC and gas chromatog. were applied as screening methods for determination of impurities in fluoxetine HCl drug substances and formulated products from multiple sources. NMR spectroscopy was also used for identification of excipients and some residual solvents. Thirty potential impurities and excipients were investigated. Several impurities were observed in generic products using gradient HPLC that were not detected with isocratic pharmacopeial methods for fluoxetine HCl. Anal. of drug substance samples and capsule formulations from many different suppliers showed a wide variation in quality which, in many cases, would go undetected using isocratic methods. The quality of the innovator's product and some generic samples was high, but many generic samples contained high levels of impurities. A new impurity, N-benzyl fluoxetine, was observed in some generic samples at levels as high as 0.9%. The gradient

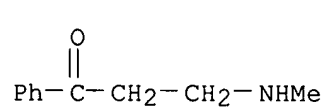
HPLC method was also used for stability studies and established that generic capsules formulated with lactose were less stable under accelerated conditions than those formulated without lactose.

IT **27152-62-1P**
RL: ANT (Analyte); **BYP (Byproduct)**; FMU (Formation, unclassified); ANST (Analytical study); FORM (Formation,, nonpreparative); **PREP (Preparation)**
(screening methods for impurities in fluoxetine HCl drug substances and formulations)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



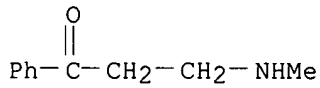
L57 ANSWER 9 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1997:684913 HCAPLUS
DN 127:283475
TI TLC examination of related substances in fluoxetine hydrochloride
AU Gao, Damin; Wang, Aimin
CS Shanghai Institute of Pharmaceutical Industry, Shanghai, 200437, Peop. Rep. China
SO Zhongguo Yiyao Gongye Zazhi (**1997**), 28(4), 175-177
CODEN: ZYGZEA; ISSN: 1001-8255
PB Zhongguo Yiyao Gongye Zazhi Bianjibu
DT Journal
LA Chinese
AB A thin layer chromatog. method to examine the related substances (ω-methylaminophenylpropanone, N-methyl-3-hydroxy-3-phenylpropane, etc) from the synthetic process of fluoxetine hydrochloride was established.

IT **27152-62-1**
RL: ANT (Analyte); ANST (Analytical study)
(determination of fluoxetine impurities by TLC)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



L57 ANSWER 10 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:741631 HCAPLUS
DN 123:338636
TI Asymmetric reactions catalyzed by chiral metal complexes. LXVI. Efficient asymmetric hydrogenation of β- and γ-amino ketone derivatives leading to practical syntheses of fluoxetine and eprozinol
AU Sakuraba, Shunji; Achiwa, Kazuo
CS School Pharmaceutical Sciences, University Shizuoka, Shizuoka, 422, Japan
SO Chemical & Pharmaceutical Bulletin (**1995**), 43(5), 748-53
CODEN: CPBTAL; ISSN: 0009-2363
PB Pharmaceutical Society of Japan
DT Journal

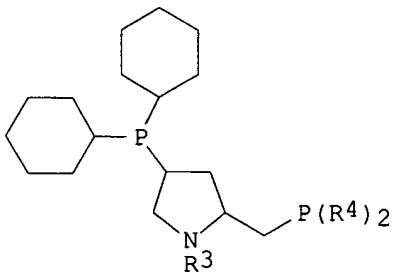
LA English
OS CASREACT 123:338636
AB N-(methylcarbamoyl)-4-(dicyclohexylphosphino)-2-[(diphenylphosphino)methyl]pyrrolidine and N-(tert-butoxycarbonyl)-4-(dicyclohexylphosphino)-2-[(diphenylphosphino)methyl]pyrrolidine rhodium(I) complexes were efficient catalysts for the asym. hydrogenation of β- and γ-amino ketone hydrochloride derivs. Utilizing this methodol., we have developed efficient syntheses of fluoxetine and eprozinol from intermediate optically active amino alcs.
IT **2538-50-3P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(asym. hydrogenation of amino ketones with rhodium complex catalysts)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



L57 ANSWER 11 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:559860 HCAPLUS
DN 119:159860
TI Preparation of optically active 3-amino-1-phenylpropanols
IN Achinami, Kazuo; Yuya, Masakazu
PA Fuji Yakuhin Kogyo Kk, Japan; Achinami Kazuo
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI JP 05070412 | A2 | 19930323 | JP 1991-310278 | 19910913 <-- |
| PRAI JP 1991-310278 | | 19910913 <-- | | |

OS CASREACT 119:159860; MARPAT 119:159860
GI



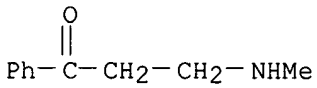
III

AB Optically active PhCH(OH)CH2CH2NR1R2 (I; R1, R2 = H, C1-4 alkyl, benzyl) mineral acid salts are prepared by asym. hydrogenation of PhCOCH2CH2NR1R2 (II; R1, R2 = same as I) mineral acid salts with metal complex catalysts containing optically active phosphinopyrrolidones (2S,4S)- or (2R,4R)-III (R3 = H, COR5, CO2R6, CONHR7; R4 = Ph optionally substituted with 1-3 groups chosen from lower alkyl, alkoxy, and dialkylamino; R5-7 = alkyl, aryl) as ligands. Chloro(1,5-cyclooctadiene)rhodium, (2S,4S)-III (R3 = Me, R4 = Ph), and II.HCl (R1 = Me, R2 = benzyl) in MeOH were stirred under 30 atm H at 50° for 48 h to give .apprx.100% (R)-I.HCl (R1 = Me, R2 = benzyl) of 90.8% ee.

IT **2538-50-3P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and stereoselective hydrogenation of)

RN 2538-50-3 HCAPLUS

CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L57 ANSWER 12 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:20725 HCAPLUS

DN 116:20725

TI Asymmetric reactions catalyzed by chiral metal complexes. XLVIII. Practical asymmetric synthesis of (R)-fluoxetine hydrochloride catalyzed by (2S,4S)-4-dicyclohexylphosphino-2-diphenylphosphinomethyl-1-(N-methylcarbamoyl)pyrrolidine-rhodium complex

AU Sakuraba, Shunji; Achiwa, Kazuo

CS Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan

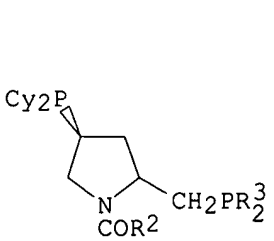
SO Synlett (**1991**), (10), 689-90
CODEN: SYNLES; ISSN: 0936-5214

DT Journal

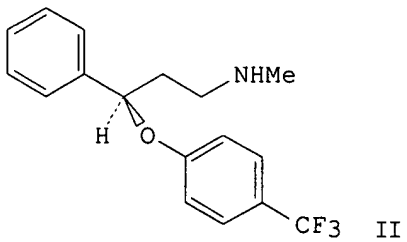
LA English

OS CASREACT 116:20725

GI



I



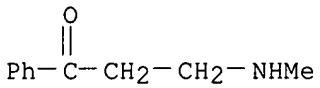
II

AB Asym. hydrogenation of PhCOCH2CH2NRR1 (R = CH2Ph, H, R1 = Me) in the presence of Rh catalysts, [Rh(COD)Cl]2-(2S,4S)-I (COD = cycloocta-1,4-diene) I (R2 = NHMe, R3 = Ph, 3,5-MeC6H3, Cy = cyclohexyl; R2 = OCMe3, R3 = Ph, Cy = cyclohexyl), gave PhCH(OH)CH2CH2NRR1.HCl with R-configuration at the hydroxy carbon. Through this procedure (R)-fluoxetine II was prepared

IT **2538-50-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydrogenation of, in presence of rhodium catalyst)

RN 2538-50-3 HCAPLUS

CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



L57 ANSWER 13 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:5913 HCAPLUS

DN 114:5913

TI Synthesis of tritium labeled 1-(3,4-dichlorophenyl)-3-(methylamino)propanol hydrochloride

AU Hill, John A.; Wisowaty, James C.

CS Chem. Dev. Lab., Burroughs Wellcome Co., Research Triangle Park, NC, 27709, USA

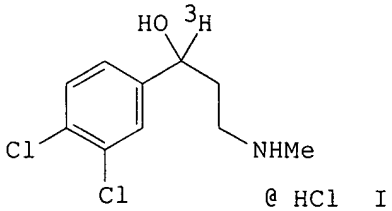
SO Journal of Labelled Compounds and Radiopharmaceuticals (**1990**), 28(7), 811-18
CODEN: JLCRD4; ISSN: 0362-4803

DT Journal

LA English

OS CASREACT 114:5913

GI

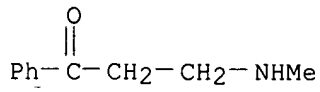


@ HCl I

AB 1-(3,4-Dichlorophenyl)-3-(methylamino)-1-propanol hydrochloride, a potential antidepressant, was synthesized by a two-step method in the [3H]-labeled form I with specific activity 12.5 mCi/mmol suitable for drug metabolism and disposition studies.

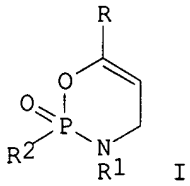
IT **2538-50-3P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**

(preparation of)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



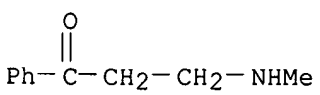
● HCl

L57 ANSWER 14 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1985:166839 HCAPLUS
DN 102:166839
TI Synthesis of heterocyclic compounds: part XXVI - 3,6-diaryl-3,4-dihydro-1,3,2-oxazaphosphorin 2-oxides
AU Modak, A. S.; Gogte, V. N.; Tilak, B. D.
CS Natl. Chem. Lab., Pune, 411 008, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (**1984**), 23B(10), 907-13
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English
OS CASREACT 102:166839
GI

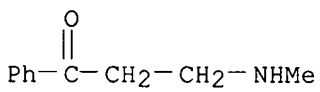


I

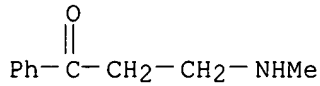
AB Cyclization of RCOCH2CH2NHR1 (R = Ph, 2-naphthyl 2-thienyl p-anisyl, p-O2NC6H4; R1 = Ph, p-anisyl, Me, o-, p-tolyl, o-, p-ClC6H4) with POCl3 gave 23-78% 20 I (R2 = Cl), which were aminated to give I (R2 = Et2N, morpholino, aziridino, piperidino, EtNH, NH2).
IT **27152-62-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with phosphorus oxychloride)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



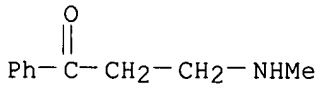
L57 ANSWER 15 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1983:405293 HCAPLUS
DN 99:5293
TI (Aminomethyl)acetophenone derivatives and their biological properties
AU Agababyan, A. G.; Gevorgyan, G. A.; Tumadzhyan, A. E.; Melkonyan, Zh. S.; Durgaryan, L. K.; Azlivyan, A. S.; Apoyan, N. A.; Mndzhoyan, O. L.
CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SO Khimiko-Farmatsevticheskii Zhurnal (**1983**), 17(3), 303-8
CODEN: KHFZAN; ISSN: 0023-1134
DT Journal
LA Russian
AB 4-RC6H4COCH2CH2NHCH(CO2H)CH2C6H4R1-4·HCl (R = H, PrO, Br, NO2, MeO, EtO; R1 = H, OH), 4-RC6H4COCH2CH2NMeCH2CO2R1·HCl (R = H, Br, Cl, Ph; R1 = H, Et), and 4-PhC6H4COCH2CH2NHCH2CO2Et·HCl were prepared by Mannich reactions of 4-RC6H4COMe. In several cases the free amines were also prepared Some of the compds. showed analgesic, local anesthetic, and antiinflammatory activity; the most effective ones had lower local anesthetic activity than novocain.
IT **27152-62-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Me bromoacetate)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



L57 ANSWER 16 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1983:127460 HCAPLUS
DN 98:127460
TI Vulcanization activity of β-aminoketone derivatives
AU Samodaeva, V. A.; Gridunov, I. T.; Kazakova, E. N.; Cherkasova, E. M.
CS MITKhT, Moscow, USSR
SO Kauchuk i Rezina (**1982**), (12), 19-20
CODEN: KCRZAE; ISSN: 0022-9466
DT Journal
LA Russian
AB The activity of β-alkylamino- and β-dialkylaminopropiophenone oximes, having the general formula PhC(:NOH)(CH2)2NRR1 (R = H, Me; R1 = Me), to accelerate the S vulcanization of natural rubber depends on the reactivity of oxime group and of the N atom in the amino group. The activity of the vulcanization accelerators decreases in the order: β-methylaminopropiophenone oxime [84606-61-1] > β-methylaminopropiophenone hydrochloride [**2538-50-3**] > β-dimethylaminopropiophenone oxime [1485-16-1] > β-dimethylaminopropiophenone hydrochloride [879-72-1] > acetophenone oxime [613-91-2]. The β-alkylamino- and β-dialkylaminopropiophenone oximes were prepared by reaction of β-aminoketone hydrochlorides with NH2OH.HCl.
IT **2538-50-3**
RL: USES (Uses)
(vulcanization accelerators, for natural rubber)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)

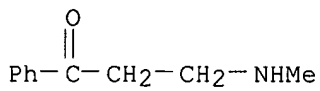


L57 ANSWER 17 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1977:72090 HCAPLUS
DN 86:72090
TI Synthesis and study of the steric structure of substituted methyl- and phenyl[2-(methylamino)ethyl]carbinols with secondary and tertiary hydroxyl groups
AU Boiko, I. P.; Zhuk, O. I.; Malina, Yu. F.; Samitov, Yu. Yu.; Unkovskii, B. V.
CS Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SO Zhurnal Organicheskoi Khimii (**1976**), 12(10), 2107-15
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
AB LiAlH4 reduction of 7 RCOCHR1CR2R3NHMe.HCl (R = Me, Ph; R1, R2, R3 = H, Me) in Et2O afforded threo- and erythro-HOCHRCHR1CR2R3NHMe in 56.8-97% yield, with the latter predominating in all cases. MeNRCH2CHMeCO2Me (I; R = H) was acetylated with Ac2O to give 83.4% I (R = Ac), which was treated with LiAlH4 or RLi (R = Me, Et, Ph) to give 50-94% MeNHCH2CHMeCR2OH (R = H, Me, Et, Ph). These compds. exist in quasi-cyclic form stabilized by an intermol. OH...N H bond.
IT **2538-50-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, with lithium aluminum hydride, configuration of products from)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)

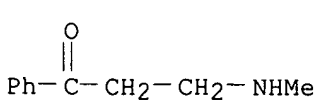


L57 ANSWER 18 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1975:442975 HCAPLUS
DN 83:42975
TI Chemistry of β-amino ketones. VII. Synthesis of substituted methyl and phenyl β-[[methyl(β-acylethyl)]amino]ethyl ketones by the aminomethylation of ketones by formaldehyde and salts of methyl and phenyl β-methylaminoalkyl ketones
AU Badosov, E. P.; Khasirdzhev, A. B.; Golovin, E. T.; Unkovskii, B. V.
CS Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR

SO Zhurnal Organicheskoi Khimii (**1975**), 11(5), 972-7
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
AB Seven PhCOCHRCH2NMeCH2R1R2COR3 (R, R1, R2 = H, Me; R3 = H, Me, Ph) were prepared in 6.35-81% yield by reaction of PhCOCHRCH2NHMe.HCl with CH2O and R3COCHR1R2. Reaction of MeCOCHMeCHMeNHMe·HCl, PhCOMe, and CH2O gave only [PhCO(CH2)2]NMe·HCl, an unexpected product.
IT **2538-50-3P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)

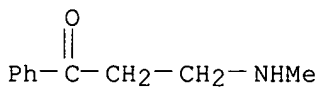


L57 ANSWER 19 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1974:403297 HCAPLUS
DN 81:3297
TI Chemistry of β-amino ketones. V. Synthesis of methyl- and phenyl-β-[N-methyl-N-(β-cyanoalkyl)amino]alkyl ketones
AU Golovin, E. T.; Badosov, E. P.; Nikiforova, A. P.; Unkovskii, B. V.
CS Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SO Zhurnal Organicheskoi Khimii (**1974**), 10(4), 706-12
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
AB MeNHCH2CH2CN added to RCOCR1:CHR2 (I; R = Me, Ph; R1, R2 = H, Me) at 20° to give 6 corresponding RCOCHR1CHR2NMeCH2CH2CN (II) in >83% yield; the reactivity of I decreased in the order RCOCH:CH2 > RCOCMe:-CH2 > RCOCH:CHMe > RCOCMe:CHMe. PhCOMe condensed with HCHO and MeNHCH2CHMeCN at 70° to give 83% PhCOCH2CH2NMeCH2CHMeCN, and MeCOCH2CMe2NHMe added to CH2:CHCN at 20° to form 19% MeCOCH2CMe2NMeCH2CH2CN; these methods gave lower yields when applied to the preparation of II.
IT **27152-62-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with acrylonitrile)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



L57 ANSWER 20 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1972:60668 HCAPLUS
DN 76:60668

TI Quantitative correlation between basicity and vulcanization activity of some β-amino ketones
AU Donskaya, M. M.; Abdel Bari, Sayed; Unkovskii, B. V.; Gridunov, I. T.
CS Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SO Kauchuk i Rezina (**1971**), 30(11), 12-14
CODEN: KCRZAE; ISSN: 0022-9466
DT Journal
LA Russian
AB Linear relations between the pKa of β-aminoketones I (R and R1 are H, Me, Et, cyclohexyl, Ph, or PhCH2; NRR1 is piperidino or morpholino) and the vulcanization time (t) of standard rubber mixes containing these accelerators have the form t = t0 + a pKa. The consts. t0 and a depend on the rubber type and other mix components. These consts. were determined for natural rubber and an isoprene rubber-butadiene-methylstyrene rubber mix.
IT **2538-50-3**
RL: USES (Uses)
(vulcanization accelerators, basicity of, vulcanization activity in relation to)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



L57 ANSWER 21 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1970:478288 HCAPLUS
DN 73:78288
TI Relation of the vulcanization activity of some phenyl β-amino ketones to their basicity
AU Unkovskii, B. V.; Donskaya, M. M.; Sayed, Abdel Bari; Gridunov, I. T.
CS Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SO Kauchuk i Rezina (**1970**), 29(7), 22-4
CODEN: KCRZAE; ISSN: 0022-9466
DT Journal
LA Russian
AB Rubber mixes containing natural rubber 100, stearic acid 0.5, ZnO 5.0, S 3.0, 2-mercaptobenzothiazole (I) 0.7, or BzCH2CH2R (II) (R = NHMe2, NHCH2Ph, NHPH, NMe2, NEt2, piperidino, or morpholino) instead of I gave excellent vulcanizates. The replacement of I with a 1:1 molar di-2-benzothiazolyl disulfide-II.HCl mixture gave vulcanizates of higher tear resistance than vulcanizates containing I. The vulcanizing activity of II increases with their pKa.
IT **27152-62-1**
RL: PROC (Process)
(rubber vulcanization in presence of, for improved tear resistance)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)

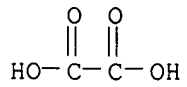
L57 ANSWER 22 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1969:460938 HCAPLUS
DN 71:60938
TI Simple synthesis of secondary Mannich bases
AU Becker, Heinz G. O.; Ecknig, W.; Fanghaenel, Egon; Rommel, S.
SO Wissenschaftliche Zeitschrift der Technischen Hochschule fuer Chemie Carl Schorlemmer Leuna-Merseburg (**1969**), Volume Date 1968, 11(1), 38-41
CODEN: WZTLA3; ISSN: 0043-6909
DT Journal
LA German
AB The H oxalates of primary and secondary amines react with a ketone and H2CO to form a Mannich base in good yield. Me2CO, MeCOEt, Et2CO, and AcPh were treated successfully with the H oxalates of MeNH2, EtNH2, and PhCH2NH2. The H oxalates of secondary Mannich bases reacted with 2 moles p-MeC6H4SO2Cl in pyridine to give the sulfonamides, which could be cleaved in 10% NaOH to the vinyl ketone and the N-substituted-p-toluenesulfonamide. The tertiary Mannich bases react with p-MeC6H4SO2NHMe in the presence of water to give the ketosulfonamides. The R1COCHR2CH2NHR3.HO2CCO2H (I) prepared are tabulated. The following R1COCHR2CH2NMeSO2C6H4Me-p (II) were prepared (R1, R2, m.p., and m.p. 2,4-dinitrophenylhydrazone given): Ph, H, 83-5°, -; Me, H, 66-8°, 145-6°; Me, Me, -(oil), 194-5°; Et, Me, -(oil), 145-6°. Even with a ten-fold excess of H2CO the formation of the normal secondary Mannich base occurs and very little of the bis product is isolated.
IT **23464-19-9P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 23464-19-9 HCAPLUS
CN Propiophenone, 3-(methylamino)-, oxalate (1:1) (8CI) (CA INDEX NAME)

CM 1

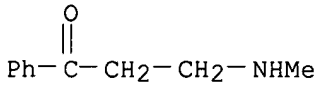
CRN 27152-62-1
CMF C10 H13 N O

CM 2

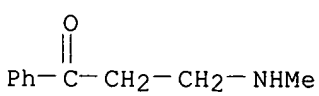
CRN 144-62-7
CMF C2 H2 O4



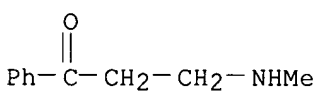
L57 ANSWER 23 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1965:15168 HCAPLUS
DN 62:15168
OREF 62:**2731b-e**
TI Preparation of Mannich bases with reversibly blocked nitrogen atom
AU Becker, H. G. O.; Fanghaenel, E.
CS Tech. Hochschule, Leuna, Merseburg, Germany
SO Journal fuer Praktische Chemie (Leipzig) (**1964**), 26(1-2), 58-66
CODEN: JPCEAO; ISSN: 0021-8383
DT Journal
LA German
OS CASREACT 62:15168
GI For diagram(s), see printed CA Issue.
AB The formation of Mannich bases from AcPh, CH2O, and amines of the trityl, benzhydryl, and tert-butyl series and the selective removal of these groups from the resulting Mannich base were studied. p-MeOC6H4CHPhNH2 (I) was converted in this manner via p-MeOC6H4CHPhNHCH2CH2Bz (II) in 60% yield into BzCH2CH2NH2 (III). p-MeOC6H4Bz (1 mole) in 200 cc. EtOH, 1 cc. AcOH, and 5 moles MeNH2 hydrogenated at 150°/140 atmospheric over 30 g. Raney Ni yielded 71% p-MeOC6H4CHPhNHMe (IV), b11 193-5°; acid oxalate m. 184°; neutral oxalate m. 206-10°. p-MeOC6H4CHNMe with p-MeOC6H4MgBr yielded 41% (p-MeOC6H4)2CHNHMe (V), b13 224°, m. 48-9°; acid oxalate m. 145°. Ph3CCl with MeNH2 yielded Ph3CNHMe, m. 73°; HCl salt m. 236°. The appropriate amine HCl salt (0.02 mole), 0.022 mole paraformaldehyde, and 20 cc. AcPh heated 0.5 hr. at 150°, and the resulting HCl salt dissolved in warm MeOH and treated with 20% aqueous NaOH yielded the corresponding free Mannich bases listed in the table. VI and VII were also prepared in 66 and 82% yield, resp., by refluxing 0.1 mole appropriate amine-HCl salt, 0.11 mole paraformaldehyde, 0.2 mole AcPh, 0.3 cc. concentrated HCl, and 30 cc. EtOH for 8 hrs. tert-Butylformimine (10 g.) and 15 g. AcPh treated with dry HCl gave 15 g. tert-BuNHCH2CH2Bz. Mannich base, Amine-HCl salt used, % yield, m.p. of HCl salt, m.p. of base; tert-BuNHCH2CH2Bz, , tert-BuNH2, 82, 206-8°, 160-1°; Ph2CHNHCH2CH2Bz (VI), Ph2CHNH2, 81, decomposed from 170, 109°; Ph2CHNMeCH2CH2Bz (VII), Ph2CHNHMe, 90, decomposed 185°, 80°; II, I, 86, 173-6°, 85; MeN(CH2CH2Bz)2, IV, 90, 165°, --; (p-MeOCH4)2CHNHCH2CH2Bz (VIII), (p-MeOC6H4)2CHNH2, 16, 168°, 104-5°; HN(CH2CH2Bz)2 (IX), --, 50, 175°, --; , MeN(CH2CH2Bz)2, V, 95, 165°, --; IX, Ph3CNH2, 95, 175°, --; MeN(CH2CH2Bz)2, Ph3CNHMe, 95, 165°, --; MeNHCH2CH2Bz, IV, 71, 164°, --; MeNHCH2CH2Bz, V, 90, 164°, --; II (0.01 mole) and 15 cc. concentrated HCl or a mixture of 7 cc. each of concentrated HCl and AcOH heated 2 hrs. in a sealed tube at 150° gave III, m. 128°, which was obtained similarly from VIII, and BzCH:CH2, b2.5 74-6°. BzCH:CH2 with PhNHNH2 yielded 1,3-diphenylpyrazoline, m. 152°. II (0.1 mole), 100 cc. 97% HCO2H, and 30 cc. 48% HBr refluxed 3 hrs. yielded 74% III.HBr, m. 144° (EtOH).
IT **2538-50-3**, Propiophenone, 3-(methylamino)-, hydrochloride
(preparation of)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



L57 ANSWER 24 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1961:2694 HCAPLUS
DN 55:2694
OREF 55:**543i,544a-c**
TI Synthesis of decahydroisoquinoline derivatives. VIII. Syntheses of 2-methyl-4-benzoyl-10-hydroxydecahydroisoquinoline and its isomer
AU Satoda, Isao; Murayama, Masao; Omoto, Toshikazu; Kawamata, Masanobu
CS Nippon Shinyaku Co., Kyoto
SO Yakugaku Zasshi (**1960**), 80, 1071-6
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Unavailable
AB cf. CA 54, 13138d. PhCOMe (120 g.), 70 g. MeNH2.HCl, and 30 g. (CH2O)n in 150 ml. EtOH heated 6 hrs. at 100-10°, the solution filtered hot, the EtOH in the filtrate removed, the residue in H2O washed with Et2O, the aqueous layer steam distilled to remove tertiary amine, the residue extracted with warm CHCl3, and concentrated gave 50 g. BzCH2CH2NHMe.HCl (I), needles, m. 141° (MeOH-Me2CO). I (5.5 g.), 2.75 g. cyclohexanone, and 2.2 g. 35% HCHO in 11 ml. H2O kept 3 days at room temperature, the mixture heated 24 hrs. at 70-80°, made alkaline with 10% NH4OH, and the product extracted with Et2O gave 8% 2-methyl-4-benzoyl-10-hydroxydecahydroisoquinoline (II), needles, m. 163-5° (Me2CO); the mother liquor yielded 26% isomer (III) of II, needles, m. 105-7°. II (1 g.) in 20 ml. Et2O at 0° stirred 1 hr. with Et2O-HCl, the precipitate filtered off, and recrystd. (EtOH-Et2O) gave 1 g. II.HCl (IV), needles, m. 280-90°. IV with cold dilute NH4OH gave II, m. 163-5°, while IV with 20% NaOH at room temperature gave III, m. 105-7°. III (1 g.) in 20 ml. Et2O at 0° stirred 1 hr. with Et2O-HCl and the product filtered off gave 1 g. III.HCl (V), needles, m. 163-4° (EtOH-Et2O). V with cold dilute NH4OH or with 20% NaOH at room temperature gave III, m. 105-7°. II (200 mg.) in 5 ml. Me2CO and 1 ml. H2O heated 20 min. on a H2O bath and cooled gave 130 mg. III, m. 105-7°. Thus, the isomers II and III were stereoisomers with different steric configuration at the 4-position.
IT **2538-50-3**, Propiophenone, 3-methylamino-, hydrochloride
(preparation of)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



L57 ANSWER 25 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1959:13099 HCAPLUS
DN 53:13099
OREF 53:**2482i,2483a-b**
TI Pharmacological and pharmacochemical studies on amino ketones
AU Nador, K.; Porszasz, J.
CS Univ. Szeged, Hung.
SO Arzneimittel-Forschung (**1958**), 8, 313-19
CODEN: ARZNAD; ISSN: 0004-4172
DT Journal
LA Unavailable
AB The following new amino ketones were prepared by Mannich reaction and tested pharmacologically (no phys. or chemical data are given): 1-piperidino-3-phenyl-3-propanone-HCl; 1-diethylamino-3-phenyl-3-propanone-HCl; 1-(2,6-dimethylpiperidyl)-3-phenyl-3-propanone-HCl; 1-piperidyl-3-(5,6,7,8-tetrahydro-2-naphthyl)-3-propanone-HCl; 1-methylamino-3-phenyl-3-propanone-HCl; 1-piperidino-3-butanone; 3-(piperidinomethyl)cyclohexanone (I); 1-(trimethylammonium)-3-butanone iodide; 2-(piperidinomethyl)decahydronaphthalen-1-one; 2-piperidino-1,2,3,4-tetrahydronaphthalen-1-one (II); N-(piperidinomethyl)phthalimide. Compds. of the general structure >NCH2CH2COR where R = aryl have an anti-nicotine effect whereas those with R = alkyl and cyclic amino ketones have a nicotine-like effect, I having the highest activity. Other compds. show adrenolytic action. II acts similarly to chlorpromazine.
IT **27152-62-1**, Propiophenone, 3-methylamino-
(pharmacology of)
RN 27152-62-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



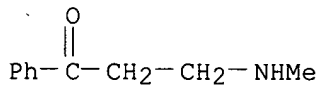
L57 ANSWER 26 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1956:45868 HCAPLUS
DN 50:45868
OREF 50:8888a-e
TI Pharmacology of amino ketones with nicotinic and anti-nicotinic effects. II
AU Porszasz, J.; Nador, K.; Gibiszer-Porszasz, K.; Wieszt, T.; Padany, R.
CS Med. Univ., Budapest
SO Acta Physiologica Academiae Scientiarum Hungaricae (**1955**), 7, 139-61
CODEN: APACAB; ISSN: 0001-6756
DT Journal
LA German
AB cf. C.A. 49, 3394i. A survey was made of the nicotinic or antinicotinic effects on blood pressure, on respiration, on the heart, and on the central nervous system, of the following compds: 1-piperidino-2-propanone, 4-(1-pyrrolidinyl)-2-butanone 4-piperidino-2-butanone, 5-piperidino-2-pentanone, 1-piperidino-4,4-dimethyl-3-pentanone, 4-piperidino-3-methyl-2-butanone, 3-(piperidinomethyl)-2-octanone, N,N-bis(2-benzoylethyl)methylamine, 1,6-dipiperidino-3,4-hexanedione, trimethyl(3-oxobutyl)aminonium iodide, (2-oxocyclopentylmethyl)diethylamine, 2-(1-pyrrolidinylmethyl)cyclopentanone, 2-(piperidinomethyl)cyclopentan

one, 2-(2-methylpiperidinomethyl)cyclopentanone, 2-(4-ethylpiperidinomethyl)cyclopentanone, 2-(cis-2,6-dimethylpiperidinomethyl)cyclopentanone, (2-oxocyclohexylmethyl)dimethylamine, (2-oxocyclohexylmethyl)diethylamine, 2-(1-pyrrolidinylmethyl)cyclohexanone, 2-(piperidinomethyl)cyclohexanone, 2-(cis-2,6-dimethylpiperidinomethyl)cyclohexanone, 4-methyl-2-(piperidinomethyl)cyclohexanone, 2-(morpholinomethyl)cyclohexanone, 2-(piperidinomethyl)-1-indanone, 3-(piperidinomethyl)camphor, octahydro-3-(piperidinomethyl)-2(1H)-naphthalenone, 2-(piperidinomethyl)-1-acenaphthenone, N,N-diethylnicotinamide, lobeline, N-benzoylethylmethylamine, 5',6',7',8'-tetrahydro-3-piperidino-2'-propionaphthone, 1-phenyl-5-piperidino-1-penten-3-one, (2-benzoylethyl)trimethylammonium iodide, (2-benzoylethyl)benzyldimethylammonium bromide, N-(2-benzoylethyl)pyrrolidine; 1-phenyl-5-pyrrolidinyl-1-penten-3-one, N-(2-benzoylethyl)-2-methyl-piperidine, N-(2-benzoylethyl)piperidine, 1-phenyl-4-piperidino-2-butanone, and parpanit.

IT **27152-62-1**, Propiophenone, 3-methylamino-
(pharmacol. of)

RN 27152-62-1 HCAPLUS

CN 1-Propanone, 3-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)



L57 ANSWER 27 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1952:2660 HCAPLUS

DN 46:2660

OREF 46:477g-i,478a-i,479a-d

TI Structural rearrangements of hydrazones

AU Theilacker, Walter; Leichtle, Otto R.

CS Tech. Hochschule, Hanover, Germany

SO Ann. (**1951**), 572, 121-44

DT Journal

LA Unavailable

GI For diagram(s), see printed CA Issue.

AB To 30 g. Ph2C:NNHPh (I) in dry Et2O were added 16 g. 70% HClO4 (II) and 27 g. Ac2O in Et2O, giving 39-40 g. II salt (III) of I, red needles, m. 186° (decomposition) (from glacial AcOH), rapidly and quantitatively hydrolyzed to I and II. When heated 9 hrs. in dry dioxane at 100°, III remained largely unchanged, giving, however, about 2 g. p-C6H4(NH2)2.2H ClO4, dark yellow, identified by conversion into the free base (IV), m. 139°, and its HCl salt. In this and subsequent rearrangements, full details are given for the separation and identification of small amts. of degradation products which in this case included BzPh, PhNHNH2, PhNH2, and NH3. When 6 g. III was heated in 100 cc. boiling PhBr, small amts. of NH4ClO4 and the II salt of IV formed (exploding, without melting between 200 and 300°) (identified by conversion into the di-Ac derivative of IV, did not m. below 290°). An unidentified violet-black amorphous substance (possibly due to oxidation of IV) was also formed. The mechanism of this p-semidine rearrangement with concomitant reduction and oxidation is discussed. p-MeC6H4NHN: CPh2 (cf. Sah and Lei, C.A. 27, 4222) yielded 70% of the II salt (V), C20H18N2.HClO4, dark red needles, m. 162° (decomposition). V heated briefly in PhBr gave resinous products, and small amts. of p-MeC6H4NH2 (identified as the HCl salt, m. 232°), NH3, traces of BzPh, but no 3,4-(H2N)2C6H3Me (showing that no o-semidine rearrangement had occurred).

To 20 g. I, 70 cc. Ac2O, and 10 g. dry ZnCl2 were added 10 cc. AcOH and 10 cc. Ac2O, the mixture warmed on a steam bath, cooled, and the filtered product washed with Ac2O and with C6H6 and dried over H2SO4, giving 30 g. of a compound (VI), C21H18ON2.ZnCl2, hygroscopic crystals, m. 214-15° which with MeOH, followed by H2O, gave Ph2C: NNAcPh (VII), m. 90-1° (from cyclohexane, followed by petr. ether), split quantitatively by concentrated HCl into PhBz and (after treatment with aqueous NaOH) PhNAcNH2, m. 119-20° (from cyclohexane). Heating VI 6 hrs. at 200-20° with excess ZnCl2, followed by treatment with MeOH gave 47% of the theoretical amount of BzPh and 30% of approx. equal parts of IV and 2-methylbenzimidazole, m. 166-8° (after sublimation). In another similar experiment, 20 g. VI (heated with 6.5 g. ZnCl2) gave 5 g. BzPh and the same bases, as well as 0.4 g. o-C6H4(NH2)2, m. 98-99°, thus indicating that both p- and o-semidine rearrangements had occurred. PhCMe:NNHPh gave an 80% (crude) yield of the II salt, yellow leaflets with greenish sheen, m. 158° (from 1:1 Et2O-AcOH); this, refluxed 0.25 hr. in PhBr, gave 4.7 g. of a mixture of NH4ClO4 and 2-phenylindole, m. 186° (from ligroine). Heating Ph2CCl2 and H2NNMe2 5 hrs., followed by Et2O extraction, washing with H2O, drying with K2CO3, and addition of II gave 63% of the II salt (VIIa) of Ph2C:NNMe2, colorless, m. 172° (readily hydrolyzed into PhBz and H2NNMe2), and 2 by-products, (Ph2CCl)2, m. 180° (cf. Finkelstein, C.A. 4, 2641), and β-benzopinacolone, m. 181°. VIIa in Me2CO with excess aqueous NaOH gave an oil, which, extracted with Et2O, gave Ph2C:NNMe2, m. 34° (from petr. ether). Molten VIIa (2 g.) heated 1 hr. at 165-170° gave only about 0.25 g. NH4ClO4, and 0.2-0.25 g. of a compound (insol. in aqueous HCl), m. 150-51° (probably 1-methyl-2-phenylisoindole, the analytical data of which were lost during the war and which up to the present has not been resynthesized); much of the original material was recovered as PhBz and Me2NNH2. PhAc and H2NNMe2 gave PhMeC: NNMe2, colorless oil not crystallizing at -15°; II salt (VIII), colorless needles, m. 107° (from EtOH), hydrolyzing slowly in moist air. When heated 2-3 hrs. at 160-70°, 60 g. VIII gave about 12.5 g. (N:CPh.CH2.CH2.N+ Me2)ClO4 (IX), m. 213-14° (by extraction with AcOH and crystallization from H2O), 6.9 g. NH4ClO4, 4.6 g. MeNH3ClO4 (isolated as the oxalate, m. 175°), 0.9 g. Me2NNH2HClO4 (isolated as the oxalate, m. 144-145°), 0.4 g. (Me2N.N:CPh.CH2.CH2)ClO4 (free base (X), m. 35-6°), 1.2 g. (Me2N.N:CPh.CH:CH)ClO4 [isolated as the HCl salt, m. 86° (free base, m. 56°; picrate, m. 130-31°)], 0.1 g. BzCH2CH2NH2.MeClO4 (m. 194-97°), and 2.4 g. dihydrodypnone, m. 72° (from MeOH). (Details of these sepns. are given.) PhMeC:NNMe2 (1.85 g.) and 4.2 g. ZnCl2 were heated 1 hr. at 200-20°, cooled, extracted with MeOH, the filtered extract poured into H2O, and the mixture filtered and treated with II, giving 0.55 g. VIII. When the above reaction was carried out with 4 (instead of 3) moles ZnCl2, 23% of the theoretical amount of VIII was formed. The following derivs. were prepared from VIII in good yields: picrate, m. 142-3° (from EtOH and dioxane); HI salt (XI), colorless leaflets, m. 220-21° (from EtOHAcOEt) (also formed from 1-methyl-3-phenylpyrazoline and MeI). The probable mechanism for the formation of IX (which contains 1 CH2 group more than VIII) is fully discussed. With 15% aqueous KOH, 3 g. IX gave BzMe and, after treatment with HCl, fractionation, and addition of (CO2H)2, the Me2NNH2 oxalate, m. 144-45° (giving a marked m.-p. depression with (MeNH)2 oxalate, m. 132°). XI carefully heated at 220-40° (at 14 mm. pressure) gave 78% X (picrate, m. 132°) (cf. K. von Auwers and Heinke, C.A. 22,422). BzCH:CH2 (0.7 g.) and 0.5 g. Me2NNH2.2HCl stirred 0.5 hr. at

100° extracted with Et2O and alc., and treated with II gave IX. IX was also formed by heating BzCH2CH2NH2.MeClO4 and Me2NNH2.2HCl at 160-70°. The following derivs. of VIII, were prepd: MeI, C11H17N2I (XII), m. 147° (decomposition); picrate of XII, m. 121°; II salt of XII, m. 145°. Dihydrodypnone semicarbazone, m. 165-6°. Me2NCH2CH2Bz (cf. Mannich and Heilner, C.A. 16, 2497) in Et2O reacted violently with MeI, giving a MeI derivative (XIII), m. 211-12° (readily split by heating with H2O into BzCH:CH2 and Me3NHI). By treatment with excess aqueous AgNO3, filtration, and addition of NaClO4, XIII gave (2-benzoylethyl)trimethylammonium perchlorate, C12H18O5NCl, m. 196-199° (decomposition) (from PhNO2). BzMe and (PhCH2)2NNH2 gave the corresponding hydrazone, C22H22N2, m. 53-54°; II salt (XIV), m. 163-65° (from PhMe). Heated 5 hrs. at 160-70° 2 g. XIV gave the following compds.: BzCH2CH2Ph, m. 70-71°; PhC:N.N(CH2Ph).CPh:CH (XV), m. 113-14°; a compound, C22H19N2Cl, m. 174-75° (not the HCl salt of either the pyrazole or pyrazoline); NH3 and (PhCH2)2NH (isolated as the HCl salt, m. 258-59°). The HCl salt of XV decomposed about 160° giving XV; the HCl salt of the 1-benzyl-3,5-diphenylpyrazoline proved unstable, and decomposed on attempted recrystn. from EtOH. By refluxing 4.3 g. 1-aminopiperidine with 5.8 g. BzMe, followed by treatment with II (at 0° in Et2O), was formed 6 g. PhCMe:NH(ClO4)N.(CH2)4.CH2, m. 124-25° (from dioxane), which, when boiled 1 hr. in PhNO2, followed by extraction with aqueous HCl, then with C6H6, and treatment (of the aqueous layer) with 40% NaOH (with subsequent, fully described purifications) gave the base, C13H16N2 or C13H14N2 (probably the latter, i.e., N:CPh.CH:C.N.CH2.CH2.CH2.CH2), m. 81° (from MeOH); picrate, m. 177°. The above rearrangements (as well as those reported by other investigators) are fully discussed. Thirty-six references.

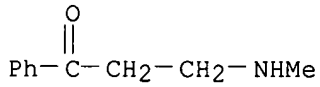
IT **857983-83-6**, Propiophenone, 3-methylamino-, perchlorate (preparation of)

RN 857983-83-6 HCAPLUS

CN Propiophenone, 3-methylamino-, perchlorate (5CI) (CA INDEX NAME)

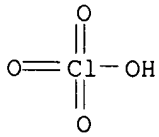
CM 1

CRN 27152-62-1
CMF C10 H13 N O

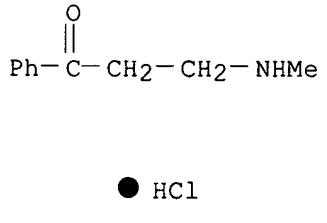


CM 2

CRN 7601-90-3
CMF Cl H O4



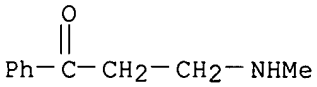
L57 ANSWER 28 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1942:12275 HCAPLUS
DN 36:12275
OREF 36:1914d-h
TI Preparation of β-keto amines by the Mannich reaction
AU Blicke, F. F.; Burckhalter, J. H.
SO Journal of the American Chemical Society (**1942**), 64, 451-4
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 36:12275
AB Equimol. amts. of PhAc and HCHO with MeNH2.HCl (Mannich and Heilner, C. A. 16, 2497) give 34 and 29%, resp., of (BzCH2CH2)2NMe.HCl (I) and BzCH2CH2NHMe.HCl (II). Steam distillation of I gives 78% of II and BzCH:CH2. Slow addition of aqueous NaOH to II in H2O at 30° gives 97% of the base of I; the intermediates are probably BzCH:CH2 and MeNH2; equimol. amts. of the two intermediates give I but no II. Compds. IIA, III, VI, VII and IX were prepared by boiling 0.1 mol of ketone, 0.1 mol of the amine-HCl, 0.12 mol of (HCHO)x and 20 cc. absolute EtOH for 2-3 h.; the mixture was cooled, the precipitate filtered and the filtrate concentrated to recover more of the desired compound; for compds. IV, V and VII, the reaction product is cooled, filtered, the solvent removed in vacuo, 50 cc. H2O added and the mixture extracted 3 times with 50-cc. portions of ether. Dimethyl-2-(2-thenoyl)ethylamine-HCl (IIA), m. 178-9°, 47%; steam distillation of IIA gives 44% of 2-thienyl vinyl ketone (IIB), b12 108-10° (PhNHNH2 gives 1-phenyl-3-(2-thienyl)pyrazoline, m. 102-3°). 1-(1-Piperidyl)-2-(2-thenoyl)ethane HCl (III), m. 201-2°, 74%. Diethyl-2-(2-thenoyl)ethyl-amine-HCl (IV), m. 116-17°, 39%; steam distillation gives IIB. Dimethyl-2-(2-thenoyl)propylamine-HCl (V), m. 154-6°, 60%; steam distillation gives 71% of 2-(2-thenoyl)propene, b19 118-20° (PhNHNH2 probably yields 1-Ph - 3 - (2 - thienyl) - 4 - methylpyrazoline, m. 81-3°). Methylbis[2-(2-thenoyl)ethyl]amine-HCl (VI), m. 185-6°; the free base m. 146-8°. Methyl(2-benzoylethyl)amine-HCl (VII), m. 140-2° 29%. Diethyl(2-benzoylethyl)amine-HCl (VIII), m. 108-10°, 45%; steam distillation gives Ph vinyl ketone, b18 114-16°. Methylbis(2-benzoylethyl)amine (IX), m. 140-1°, 34%; this results in 61% yield from Ph vinyl ketone and MeNH2 in EtOH, and in 4.7-g. yield from 8.8 g. PhAc, 3 g. (HCHO)x and 8 g. of methylacetamide-0.5HCl (m. 87-9°) in 10 cc. absolute EtOH on heating on a steam bath for 45 min. Dicyclohexylamine-HCl does not condense with HCHO and PhAc.
IT **2538-50-3**, Propiophenone, β-methylamino-, -HCl
(preparation of)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L57 ANSWER 29 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1922:14367 HCAPLUS
DN 16:14367
OREF 16:2497i,2498a-e
TI Synthesis of β-keto bases from acetophenone, formaldehyde and amine salts
AU Mannich, C.; Heilner, G.
SO Ber. (**1922**), 55B, 356-65
DT Journal
LA Unavailable
OS CASREACT 16:14367
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 15, 86 1. From 40 g. PhCOMe, 10 g. paraform and 27.5 g. NHMe2.HCl boiled in alc. is obtained 42 g. of the hydrochloride (A), leaflets from alc., needles from Me2CO, m. 156°, of ω-dimethylaminopropiophenone, b14 110-2°; oxime, tables from dilute alc., m. 108°. A (2.2 g.) decolorizes 8.8 g. KMnO4, yielding CO2, BzOH and NHMe2. Steam decomps. A into PhCOCH:CH2 and NHMe2.HCl. Hydrogenation of A in H2O with palladinized charcoal generally gave quant. the hydrochloride, leaflets from Me2CO, m. 135-6° of I-phenyl-3,3-dimethylamino-1-propanol (B), oil of a basic odor; benzoate, b15 130-60° (hydrochloride, m. 170°). In one case the reduction of A proceeded beyond the alc. stage, giving a mixture of bases b15 80-130°, separated by benzoylation by the Schotten-Baumann method into 2 fractions b15 80-100° and 100-80°; distillation of the 1st fraction under atmospheric pressure yielded PhCH2CH2CH2NMe2, b. 215-20° (methiodide, m. 175.5°; picrate, m. 103°; chloroplatinate, m. 151°). A and activated Al in Et2O gently warmed several hrs. with gradual addition of H2O yielded, besides a little B, chiefly 2 isomeric 1,6-bis[dimethylamino]-3,4-diphenylhexanediols (dl and meso-forms): α, m. 146°, and β, sinters about 100°, m. 107°. α,α'-Bis[phenylacylomethyl]methylamine (methylbis-[β-benzoylethyl]amine) (C), rodlets or needles, m. 142°, is obtained as the hydrochloride (20.5 g.), needles from alc., m. 162°, from 48 g. PhCOMe, 12 g. paraform and 14.8 g. NH2Me.HCl; the mother liquor contains a small amount of ω-methylaminopropiophenone hydrochloride (D); best prepared by distilling the preceding salt with steam, whereby PhCOCH:CH2 is also formed; D seps. from Me2CO in leaflets, m. 139-41°; it can also be obtained in 7 g. yield from 12 g. PhCOMe, 7 g. NH2Me.HCl and 3 g. paraform boiled a short time in 15 cc. alc., filtered, freed from alc. by evaporation, stirred with Et2O (which removes 5.8 g. unchanged PhCOMe) and distilled with steam. C (10 g.), reduced in Et2O with activated Al, gives 1.2 g. of a compound separating from alc. in leaflets, m. 205°, and 2 g. of an isomer, fine needles from Me2CO, sinters about 170°, m. around 180°; the compds. are probably dl- and meso-forms of the cyclic pinacol HOCPh.CH2.CH2 NMe. HOCPh.CH2.CH2
IT **2538-50-3**, Propiophenone, β-methylamino-, hydrochloride
(preparation of)
RN 2538-50-3 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

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* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d sta que l70
L68             STR
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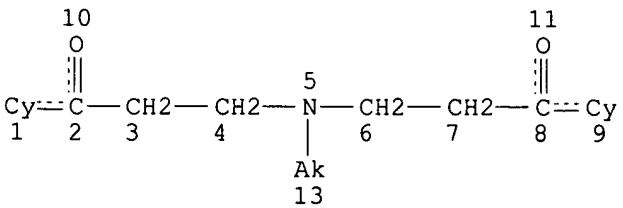

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L70          68 SEA FILE=REGISTRY CSS FUL L68

100.0% PROCESSED  306517 ITERATIONS                          68 ANSWERS
SEARCH TIME: 00.00.08


=> d his l70-

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L70          68 S L68 CSS FUL
                SAV TEMP L70 SHA525D/A

     FILE 'HCAPLUS' ENTERED AT 09:26:11 ON 23 MAY 2006
L71           6 S L70 AND L59
L72           3 S L63 AND L71
L73           5 S L62,L72 AND L58-L65,L71,L72

     FILE 'REGISTRY' ENTERED AT 09:26:55 ON 23 MAY 2006

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 09:27:04 ON 23 MAY 2006
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FILE COVERS 1907 - 23 May 2006  VOL 144 ISS 22
FILE LAST UPDATED: 22 May 2006  (20060522/ED)

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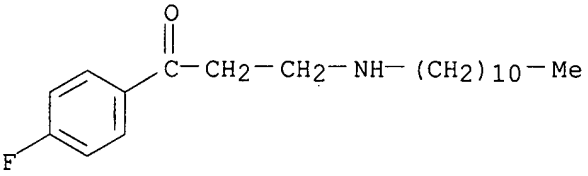
 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d l73 bib abs hitstr retable tot

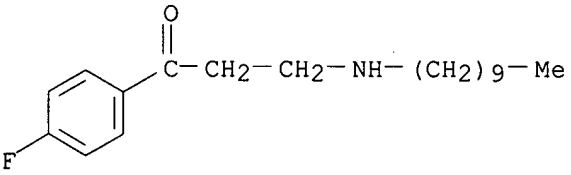
L73  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2006 ACS on STN
```

AN 1993:101592 HCAPLUS
DN 118:101592
TI Antiinflammatory phospholipase-A2 inhibitors. II. Design, synthesis and structure-activity relationship.
AU Wilkerson, W.; DeLucca, I.; Galbraith, W.; Kerr, J.
CS DuPont **Merck** Pharm. Co., Wilmington, DE, 19880-0353, USA
SO European Journal of Medicinal Chemistry (**1992**), 27(6), 595-610
CODEN: EJMCA5; ISSN: 0223-5234
DT Journal
LA English
AB The design and synthesis of a novel series, RX(CH2)nC(Y)R1 (R = dodecyl, undecyl, tridecyl, hexyl, heptyl, octyl, 1-, 2-naphthylethyl, 4-MeC6H4, 4-pyridyl, dehydroabietyl, etc.; X = NH, NEt, S, CH2, n = 2, 3, Y = H,OH, H,NH, O, MeON, R1 = H, Me, hexyl, 4-FC6H4, 4-MeOC6H4, 4-MeSC6H4, etc), of phospholipase-A2 (PLA2) inhibitors with antiinflammatory activity was based on a systematic structure-activity relationship anal.
IT **132427-66-8P 132427-67-9P 145878-92-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation and antiinflammatory activity of)
RN 132427-66-8 HCAPLUS
CN 1-Propanone, 1-(4-fluorophenyl)-3-(undecylamino)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

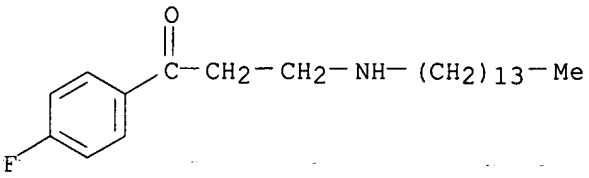
RN 132427-67-9 HCAPLUS
CN 1-Propanone, 3-(decylamino)-1-(4-fluorophenyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

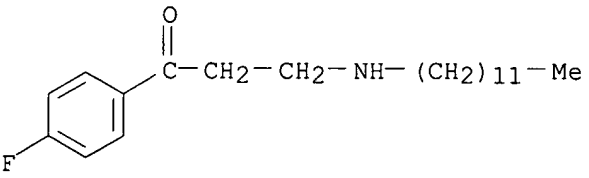
RN 145878-92-8 HCAPLUS
CN 1-Propanone, 1-(4-fluorophenyl)-3-(tetradecylamino)-, hydrochloride (9CI)

(CA INDEX NAME)



● HCl

IT **132427-58-8P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation, reduction or oximation, and antiinflammatory activity of)
RN 132427-58-8 HCAPLUS
CN 1-Propanone, 3-(dodecylamino)-1-(4-fluorophenyl)-, hydrochloride (9CI)
(CA INDEX NAME)

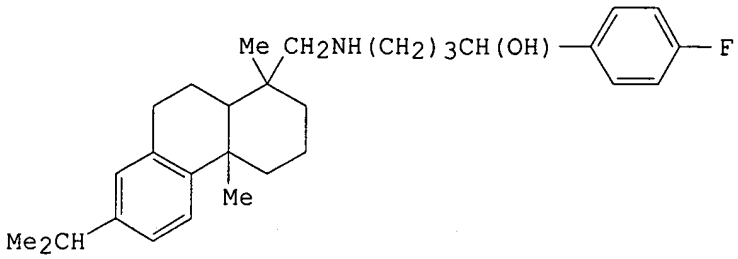


● HCl

L73 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:6747 HCAPLUS
DN 118:6747
TI Benzyl alcohol phospholipase A2 inhibitors
IN Wilkerson, Wendell W.
PA Du Pont **Merck** Pharmaceutical Co., USA
SO U.S., 15 pp. Cont.-in-part of U.S. Ser. No. 126,617, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI US 5124334 | A | 19920623 | US 1989-387319 | 19890728 <-- |
| PRAI US 1987-126617 | B2 | 19871130 <-- | | |

OS MARPAT 118:6747
GI

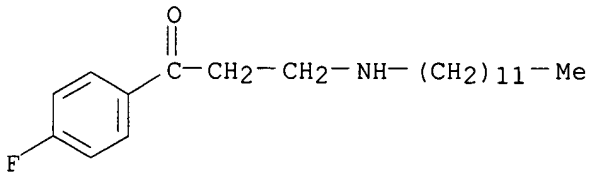



I

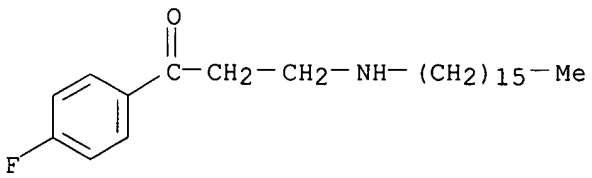
AB The present invention consists of title compds. RX(CH2)nCH(OH)C6H4Z (Z = H, F, Cl, Br, OR1, S(O)mR1; R1 = H, Me, Et, m = 0, 1, 2; n = 2, 3; X = NH, O; R = C7-25 alkyl, pyridyl, benzhydryl, phenyl(4-pyridyl)methyl, C7-25 alkaryl, substituted alkaryl where the substitution is on the aromatic moiety and is F, Cl, Br, OR3, S(O)rR3, C1-10 alkyl, R3 = Me, Et, r = 0, 1, 2; provided that when X = O, n = 3), a pharmaceutically acceptable salt, pharmaceutical compns. containing them, and methods of treating phospholipase A2-mediated conditions in mammals by administration of a therapeutically effective amount of such a benzyl alc. phospholipase inhibitors. The title compds. are useful as inflammation inhibitors. Thus, a mixture of 4-chloro-4'-fluorobutyrophenone-2,2-dimethylpropylene ketal, dehydroabietylamine, K2CO3, and KI in DMF was stirred at reflux for 24 h and concentrated to give an oil which was treated with concentrated HCl in MeOH and then 2 N NaOH followed by 4-MeC6H4SO3H. The resulting amino ketone was reduced with NaBH4 in 2:1 THF/isopropanol and converted to the HCl salt to give 76% [[[dimethyloctahydropropylphenanthrenyl]methylamino]propyl]fluoro benzenemethanol hydrochloride I. Application of I to the ears of mice reduced tetradecanoyl phorbol acetate-induce swelling by 57%.

IT **143667-19-0 143667-20-3 143667-21-4 143667-22-5 143667-27-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in synthesis of benzyl alc. phospholipase A2 inhibitors)

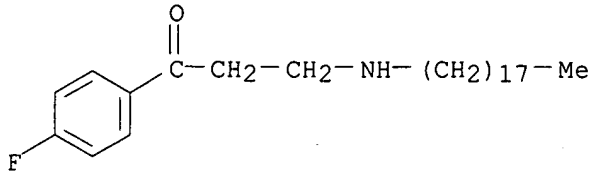
RN 143667-19-0 HCAPLUS
CN 1-Propanone, 3-(dodecylamino)-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



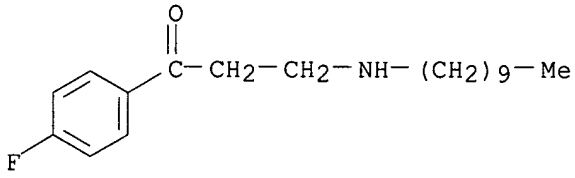

RN 143667-20-3 HCAPLUS
CN 1-Propanone, 1-(4-fluorophenyl)-3-(hexadecylamino)- (9CI) (CA INDEX NAME)



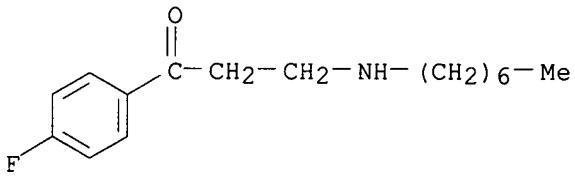
RN 143667-21-4 HCAPLUS
CN 1-Propanone, 1-(4-fluorophenyl)-3-(octadecylamino)- (9CI) (CA INDEX NAME)



RN 143667-22-5 HCAPLUS
CN 1-Propanone, 3-(decylamino)-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

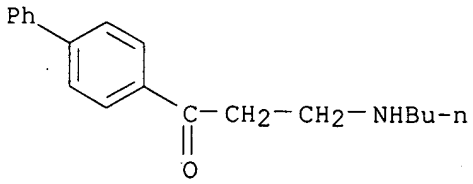


RN 143667-27-0 HCAPLUS
CN 1-Propanone, 1-(4-fluorophenyl)-3-(heptylamino)- (9CI) (CA INDEX NAME)

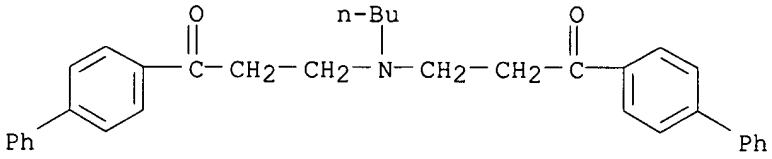


L73 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1973:478308 HCAPLUS
DN 79:78308
TI Reaction of aryl vinyl ketones with nucleophilic reagents
AU Stepanovicius, J.; Vaitkevicius, A.; Palubinskas, V.; Dienys, G.
CS Vil'nyus. Gos. Univ., Vilnius, USSR
SO Sin. Izuch. Fiziol. Aktiv. Veshchestv, Mater. Konf. (**1971**), 93-6
Publisher: Vil'nyus. Gos. Univ., Vilnyus, USSR.
CODEN: 26YYAS
DT Conference
LA Russian
AB Reaction of 4-PhC6H4COCH:CH2 with HO- and PhO- gave 58% 4-PhC6H4COCH2CH2OH and 65% 4-PhC6H4CO(CH2)2OPh, resp. Reaction of CH2:CHCOR(I; R = 4-PhC6H4, 4-MeC6H4, 4-BrC6H4) with S2- gave 50-88% [RCO(CH2)2]2S. When the nucleophile was R1S- (R1 = 4-MeC6H4, Bu) 44-79% RCO(CH2)2SR1 (R = 4-MeOC6H4, 4-MeC6H4, 4-PhC6H4, Ph, 4-BrC6H4) were obtained. Reaction of BuNH2 with I (R = 4-PhC6H4) gave 64% 4-PhC6H4CO(CH2)2NHBu; addition of I gave 53% [4-PhC6H4CO(CH2)2]2NBu. Similar results were obtained with NH3 and R2NHNH2 (R2 = H, Me, Ph, 2,4-(O2N)2C6H3, CONH2).
IT **42537-35-9P 42575-21-3P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 42537-35-9 HCAPLUS

CN 1-Propanone, 1-[1,1'-biphenyl]-4-yl-3-(butylamino)- (9CI) (CA INDEX NAME)



RN 42575-21-3 HCAPLUS
CN 1-Propanone, 3,3'-(butylimino)bis[1-[1,1'-biphenyl]-4-yl- (9CI) (CA INDEX NAME)

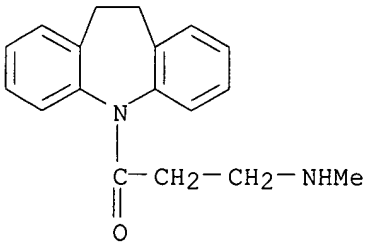


L73 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1968:419000 HCAPLUS
DN 69:19000
TI The synthesis and pharmacological study of acyl derivatives of iminodibenzyl
AU Bagal, V. N.; Kvitko, I. Ya.; Lapin, I. P.; Porai-Koshits, B. A.; Favorskii, O. V.
CS Leningr. Tekhnol. Inst. im. Lensoveta, Leningrad, USSR
SO Khimiko-Farmatsevticheskii Zhurnal (**1967**), 1(12), 21-6
CODEN: KHFZAN; ISSN: 0023-1134
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB The treatment of 10,11-dihydro-5H-dibenz[b,f]azepine (I) with halopropionyl chlorides and subsequently with primary or secondary amines, afforded II and IIa, resp. Treating 2 g. I and 1.3 g. freshly distilled ClCH2CH2COCl in anhydrous C6H6 gave 2.37 g. N-(β-chloropropionyl)-10,11-dihydro-5H-dibenz[b,f]azepine (III), m. 105-6° (EtOH). Similarly, 7.5 g. I and 7.4 g. BrCH2CHMeCOCl gave 11.8 g. N-(β-bromo-α - methylpropionyl) - 10,11 - dihydro-5H - dibenz[b,f]azepine, m. 118.5° (cyclohexane). A solution of 2.85 g. III in 70 ml. anhydrous PhMe was treated with 2.02 g. iso-Pr2NH, the mixture refluxed 18 hrs., the solid removed, and the filtrate evaporated to give an oily residue which was dissolved in anhydrous Et2O and treated with HCl-saturated Et2O to give 1.7 g. II
(R = H, R' = R" = iso-Pr, X = HCl) (IIb), m. 187-8° (iso-PrOH). Analogously were prepared the following II (R, R', R", X, m.p., and % yield given): H, H, Me, HCl, 167° (decomposition) (EtOH), 20; H, Me, Me, HCl, 165-7° (EtOH-Et2O), 87; H, Et, HCl, 168-70° (EtOH-Et2O), 40; H, Bu, Bu, (CO2H)2, 126-7° (EtOH-Et2O), 54.5; H, Me, Ph, HCl, 172-4° (iso-PrOH), 33; (CH2)2OH, PhCH2, (CO2H)2, 170-2° (EtOH), 75; Me, Me, Me, HCl, 240-1° (MeOH), 43; Me, Et, Et, HCl, 230-1° (MeOH), 52; H, H, (CH2)2OCH2Ph, -, 101-3°, -. Also prepared were the following IIa (R, R', X, m.p., and % yield given): H,

4-morpholinyl, HCl, 205-6° (EtOH), 54.6; H, 1-methyl-4-piperazinyl, HCl, 227-32° (EtOH), 83; H, 1-(β-hydroxyethyl)-4-piperazinyl, 2HCl (IIc), 130° (iso-PrOH), 51; H, 1-piperidinyl, HCl, 158-9° (iso-PrOH), 67.5; Me, 1-piperidinyl, HCl, 248° (iso-PrOH), 50; Me, 4-morpholinyl, HCl, 250-1° (iso-PrOH), 39. A 1:1 mixture of III and N-(β-hydroxyethyl)piperazine gave IV, m. 238-8.5° (MeOH), as opposed to a 1:6 mixture which gave only IIc. A solution of 0.85 g. III in 15 ml. anhydrous C6H6 was treated with 0.75 g. MeNH2 in 5 ml. C6H6, the mixture kept 7 days, refluxed 2 hrs., the solid removed, the filtrate worked up as for IIb to give an oily product which was dissolved in an alc. and precipitated with petroleum ether to give 0.5 g. V, m. 137° (decomposition). The reaction of 2.85 g. III and 2.67 g. N-methylpyridone gave 1.25 g. N-acryloyl-10,11-dihydro-5H-dibenz[b,f]azepine, m. 97-8° (iso-PrOH). The compds. exhibited adrenopos., cholinoneg., and antireserpine action in rats and mice.

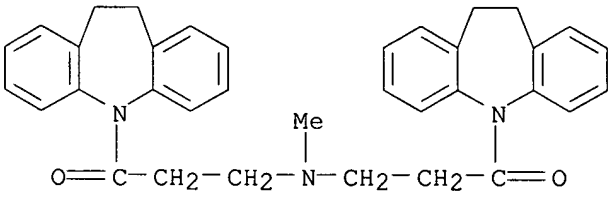
IT **19055-28-8P 19290-18-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

RN 19055-28-8 HCAPLUS
CN 5H-Dibenz[b,f]azepine, 10,11-dihydro-5-[3-(methylamino)-1-oxopropyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 19290-18-7 HCAPLUS
CN 5H-Dibenz[b,f]azepine, 5,5'-[(methylimino)bis(ethylenecarbonyl)]bis[10,11-dihydro-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

L73 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1967:46298 HCAPLUS
DN 66:46298

TI Spatial structure and stereochemistry of synthesis of 1-alkyl-4-phenyl-3-benzoyl-4-piperidols

AU Unkovskii, B. V.; Mel'nikova, A. A.; Zaitseva, M. G.; Malina, Yu. F.
CS M. V. Lomonosov Fine Chem. Tech. Inst., Moscow, USSR

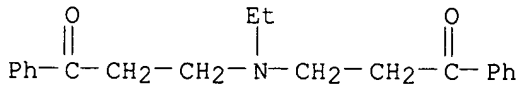
SO Zhurnal Organicheskoi Khimii (**1966**), 2(8), 1501-7
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian

GI For diagram(s), see printed CA Issue.

AB Cyclization of bis(2-benzoylethyl)alkyl amines in basic medium led to stereospecific formation of but one of two possible geometrical isomers of 1-alkyl-3-benzoyl-4-phenyl-4-piperidols; this one had the cis-configuration and predominant conformation of 3-equatorial-4-axial-disposition of Bz and OH groups, resp., as indicated by examination of the ir spectra. The ketones were prepared previously (Plati and Wenner, (CA 43, 9050b). Heating 47.2 g. AcPh with 12 g. paraformaldehyde and 19.1 g. PrNH2.HCl to 85° gave after cooling BzCH2CH2NHPr.HCl, m. 125-7°, which in aqueous NaOH in 0.5 hr. at room temperature gave 58% 1-propyl-4-phenyl-3-benzoyl-4-piperidol, m. 101-2°. Similar reaction with other RNH2 gave exclusively RN(CH2CH2Bz)2.HCl which in basic medium cyclized as above. The following were reported: 95% EtN(CH2CH2Bz)2.HCl (I), m. 126-7°; 89% BuN analog of I m. 62-4°; 91.5% PhCH2N analog of I, m. 122.5-3.5°; 51% 1-ethyl-4-phenyl-3-benzoyl-4-piperiodol (II), m. 99.5-100.5°; 67.5% 1-butyl analog of II, m. 95-6°; 89.5% 1-benzyl analog of II, m. 116.5-17.5°. Ir spectra are shown.

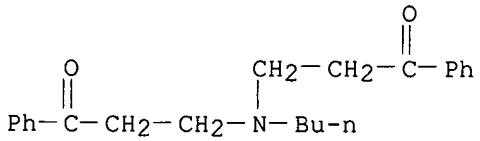
IT **13721-12-5P 13721-13-6P 13734-99-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

RN 13721-12-5 HCAPLUS
CN 1-Propanone, 3,3'-(ethylimino)bis[1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

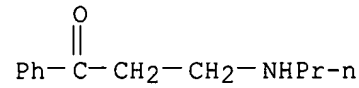
RN 13721-13-6 HCAPLUS
CN 1-Propanone, 3,3'-(butylimino)bis[1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 13734-99-1 HCAPLUS

CN Propiophenone, 3-(propylamino)-, hydrochloride (8CI) (CA INDEX NAME)



● HCl

=> => d his l1-l73

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L1             1 S (WO2003-EP8514 OR DE2002-10240026)/AP,PRN
                 E FABIAN/AU
                 E FABIAN K/AU
L2            24 S E3-E5
                 E NIESERT/AU
L3            15 S E7-E9
                 E KRALIK/AU
L4            30 S E33-E35,E42
                 E GLUSENKAMP/AU
L5             6 S E4,E5
                 SEL RN L1

     FILE 'REGISTRY' ENTERED AT 08:56:37 ON 23 MAY 2006
L6             4 S E1-E4
L7             2 S L6 NOT (CH2O OR C6H6OS)
L8             3 S 27152-62-1/CRN
L9             6 S 667465-15-8/CRN
L10            3 S L9 NOT COMPD
L11            8 S L7,L8,L10
L12              STR
L13            1 S L12 CSS SAM
L14              SCR 1597
L15            8 S L12 AND L14 CSS SAM
L16          570 S L12 AND L14 CSS FUL
                 SAV TEMP L16 SHA525/A
L17           21 S L16 AND SC4/ES
L18           15 S L17 AND 1/NR
L19            6 S L17 NOT L18
                 SEL RN 4-6
L20            3 S L19 NOT E5-E7
L21           18 S L18,L20
L22          239 S L16 AND 46.150.18/RID
L23          169 S L22 AND 1/NR
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L25           10 S L24 CSS SAM SUB=L16
L26          297 S L24 CSS FUL SUB=L16
                 SAV TEMP L26 SHA525A/A
L27          296 S L26/COM
L28           19 S L17 AND L27
L29            1 S L28 NOT L21
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L30          18 S L28 NOT L29
L31          18 S L21,L30
L32         128 S L27 AND 46.150.18/RID
L33         112 S L32 AND 1/NR
L34         111 S L33 NOT MAN/CI
L35         129 S L31,L34
L36          15 S L32 NOT L35
L37          14 S L36 NOT MAN/CI
L38         143 S L35,L37
L39             STR L24
L40           4 S L39 CSS SAM SUB=L27
L41         158 S L39 CSS FUL SUB=L27
                SAV TEMP L41 SHA525B/A
L42         272 S L38,L41
                SAV TEMP L42 SHA525C/A
L43          25 S L26 NOT L42
L44         264 S L42 NOT L11

     FILE 'HCAOLD' ENTERED AT 09:16:27 ON 23 MAY 2006
L45           3 S L11
                SEL AN
                EDIT E8-E10 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 09:16:55 ON 23 MAY 2006
L46           6 S E8-E10
L47           3 S L46 NOT (CARLIN ? OR SOKOLOV ? OR GRAFE ?)/AU
L48          36 S L11
L49          36 S L47,L48
L50          29 S L49 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L51           2 S L49 AND L1-L5
L52           2 S L49 AND MERCK?/PA,CS
L53          18 S L11(L)PREP+NT/RL
L54          12 S L50 AND L53
L55          13 S L51,L52,L54
L56          16 S L50 NOT L55
L57          29 S L55,L56

     FILE 'REGISTRY' ENTERED AT 09:19:56 ON 23 MAY 2006

     FILE 'HCAPLUS' ENTERED AT 09:20:39 ON 23 MAY 2006
L58         106 S L44
L59         101 S L58 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L60           0 S L58 AND L1-L5
L61           2 S L58 AND MERCK?/PA,CS
L62           2 S L59 AND L61
L63          64 S L44 (L) PREP+NT/RL
L64          59 S L59 AND L63
L65          60 S L62,L64

     FILE 'REGISTRY' ENTERED AT 09:23:33 ON 23 MAY 2006

     FILE 'HCAPLUS' ENTERED AT 09:23:36 ON 23 MAY 2006
L66             TRA L65 1- RN :     3115 TERMS

     FILE 'REGISTRY' ENTERED AT 09:23:38 ON 23 MAY 2006
L67         3115 SEA L66
L68             STR
L69           0 S L68 CSS
L70          68 S L68 CSS FUL
                SAV TEMP L70 SHA525D/A
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     FILE 'HCAPLUS' ENTERED AT 09:26:11 ON 23 MAY 2006
L71             6 S L70 AND L59
L72             3 S L63 AND L71
L73             5 S L62,L72 AND L58-L65,L71,L72

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